Indian J. Phys. **69A** (1), 53 – 64 (1995)

IJP A
— an international journal

Electron Correlation and Magnetism: a perspective

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Abstract

A brief survey of the present status of the correlation problem in metals, particularly of results on single band Hubbard model, for nonexperts, is given.

Keywords. Electron correlations, Magnetism, Hubbard Model,

PACS Nos. 71.27.+a, 71.30.+h, 75.10 Lp

1 Introduction

Most of the magnetic properties of solids arise from electrons and their mutual interactions. In fact the origin of Hund's rule, which says that the ground state of an atom has maximum multiplicity, and which is responsible for atomic magnetic moments, lies in the reduction in energy due to the exchange part of the electron-electron interaction. In solids, the phenomenon of magnetism has to be understood by quantum many body considerations of the electron-electron interaction. In this article, which is essentially a verbatim report of my talk given at CMP94 meeting at Calcutta, we present a panoramic view of the results on the correlation effects in metals. In the first two sections we give the scope of the subject of magnetism and talk about the necessity of inclusion of correlation in the free electron theory of metals. We then introduce some minimal models of correlation and magnetism in solids. Finally we present a brief perspective of some old and recent results on the Hubbard model. One comment about the reference list, it can be made longer than the text. Rather, it is given to provide suggestions for additional reading related to the problems and questions which are only flashed here.

2 Magnetism

The subject of magnetism deals with the behavior of materials in the presence of a magnetic field. Materials are usually classified as diamagnets, paramagnets or magnets with some ordered magnetic moments, depending on whether they expel or attract the magnetic lines of force, or whether they exhibit some kind of spontaneous ordering of magnetic moments below a certain temperature. This behaviour can be due to intrinsic atomic moments or due to spin and orbital degrees of freedom of conduction electrons. In particular, the orbital degree of freedom is responsible for the de Haas-van Alphen effect and many galvanomagnetic properties of metals. It is also responsible for the Meissner effect in superconductors and for the fractional and the integer Quantum Hall effect in the inversion layer formed in Mosfet heterostructure devices [1].

Instead of the bulk magnetic properties, we can put a magnetic impurity in a solid to see what happens. The result of course depends on the type of the host matrix. For example, in insulators when the rotation symmetry of moment is incommensurate with that of the host lattice, it results in a crystal field splitting of atomic levels of the impurity. In some semiconductors, (e.g. $Pb_{1-x}Mn_xTe$), the moment gets enhanced because of the formation of a bound magnetic polaron [2]. In metals, the spin density of conduction electrons shows Friedel oscillations around the impurity and also there is a possibility of complete moment suppression due to screening (Kondo effect) [3]. In superconductors, the magnetic impurity can suppress T_c, lead to the phenomenon of gapless superconductivity, or a reentrance behavior due to interplay of magnetic and superconductive correlations in some materials [4].

To have an ordered magnetic lattice, the magnetic moments must interact, either amongst themselves or with conduction electrons, or as it happens in some metals, the electron-electron interaction itself is strong enough to give rise to a magnetic order [5]. Apart from the magnetic order, there is also a possibility of enhancement of equilibrium properties, like electronic specific heat, by an enormous amount because of the interaction between electrons and local orbitals. This happens in some rare earth compounds, (e.g. $CeAl_3$, and UPt_3), known as heavy fermion materials [6]. They exhibit many interesting properties which have not been understood so far.

Finally we can have a lattice of magnetic fields (flux lattice). This happens in type II superconductors. An understanding of the phenomenon of pinning and melting of the flux lattice can lead to better technological applications of recently discovered high temperature superconductors [7].

3 Electron Correlations

The nearly free electron model has been a very useful model of metals. Much of the thermal, optical and transport behaviors of metals can be described within this model once either conduction electron density, or the Fermi temperature or the density of states at the Fermi energy is known. The success of this model in real metals lies in the existence of a weak pseudopotential in which the electrons move. However, the model is featureless: it does not show magnetism, nor superconductivity, nor explains the insulating behavior of some half-filled band materials (e.g. NiO) or the metal-insulator transition in some of them, e.g. in $(V, Cr)_2O_3$. It is also not possible to understand the phenomenon of moment formation (or suppression) in metals [3], or the large effective mass of electrons in some rare earth materials (heavy fermions) or for that matter the fractional Quantum Hall effect [1]. There are mainly two reasons. The first is that the interaction of electrons with other degrees of freedoms in the solid has been ignored. For example, the interaction with lattice vibrations has been known to give rise to superconductivity in many metals. The second reason is that the Coulomb interaction amongst electrons themselves has been ignored. Some aspects of this interaction are well understood, for example the screening and plasma oscillation in normal metals. However, in transition metals, rare earths and actnides, one is dealing with partially filled narrow d- or f- bands. The effective interaction is qualitatively different. For narrow bands, the electron-electron interaction is large only when the electrons encounter each other on the same ionic site, consequently the range of effective interaction gets shortened and the strength enhanced. Instead of treating the effects of long range Coulomb force properly, which is very difficult, some kind of model building is done. We now present some models of strongly correlated electrons and of magnetism.

4 The Minimal Models

1. Hubbard Model: This model was introduced independently by Gutzwiller, Hubbard, and by Kanamori in early sixties [8]. It has the nearest neighbour hopping of conduction electrons as the kinetic energy term and approximates an effective short range interaction with a zero range intra-atomic Coulomb term In the usual notation, it is given by,

$$H = \sum_{i,j} t_{i,j} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} \tag{1}$$

Though the model considers the Coulomb term in an extremely simplified form, it seems to contain the essential physics of narrow band metals. It has been used to explain the metal-nonmetal transition in some transition metal oxides, magnetism in metals, low temperature behavior of liquid ^{3}He and superconductivity in cuprates [8, 9].

2. Anderson Model: In this model a magnetic impurity is described by a localized extra d-orbital which is located in the conduction band of host. The interaction with the conduction electrons is described by a mixing term which leads to a broadening of the impurity level corresponding to a resonance state or "virtual bound state" [10].

$$H = \sum_{k,\sigma} \epsilon_{k,\sigma} a^{\dagger}_{k,\sigma} a_{k,\sigma} + E c^{\dagger}_{\sigma} c_{\sigma} + U n^{c}_{\uparrow} n^{c}_{\downarrow} + \sum_{k,\sigma} \{ V_k a^{\dagger}_{k,\sigma} c_{\sigma} + (H.c) \}. \tag{2}$$

During the last three and half decades it has been used to explain behavior of magnetic moment in a metal, suppression and formation of moments, and the phenomenon of valence fluctuations in rare earth impurities ($CeSn_3$, $TmSe$). The well known s-d exchange model can be derived from this model using a canonical transformation (Schrieffer-Wolf transformation).

3. Periodic Anderson Model: This is an extension of previous model for a lattice of atomic orbitals in a sea of conduction electrons.

$$\begin{aligned} H &= \sum_{k,\sigma} \epsilon_{k,\sigma} a^\dagger_{k,\sigma} a_{k,\sigma} + \sum_{i,\sigma} E_\sigma c^\dagger_{i,\sigma} c_{i,\sigma} + U \sum_i n^c_{i,\uparrow} n^c_{i,\downarrow} \\ &+ \frac{1}{\sqrt{N}} \sum_{k,i,\sigma} \{V_k e^{i\mathbf{k}\cdot\mathbf{R}_i} a^\dagger_{k,\sigma} c_{i,\sigma} + (H.c)\}. \end{aligned} \tag{3}$$

In principle the physics of transition metals, rare earths, and actinide metals is described by this model. Here we have a narrow band embedded in a broad conduction band. However, with varied degree of success, it has been applied to mixed valence compounds, heavy fermions ($CeCu_6$, U_2Zn_{17}), and at present to Kondo insulators ($Ce_3Bi_4Pt_3$, $CeNiSn$) [11].

4. Heisenberg Model: This is one of the earliest models of magnetism in solids. It is appropriate for insulators. However, it is difficult to derive in realistic situations.

$$H = \sum_{i,j}{}' J_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j . \tag{4}$$

It has also been a starting point of many calculations in statistical physics In particular the Ising model, and the X-Y model are special cases of it.

We have introduced the minimal models. They contain a very limited aspect of the real correlation problem. For example, the long range nature of Coulomb force which is important in the insulating side of the metal to insulator transition and which is also responsible for the charge density wave formation has not been considered. Similarly the orbital degeneracy, anisotropy, dipolar forces, disorder and interaction with other degrees of freedon have not been considered. These are very important for detailed studies of the correlation problem in real solids. Now for rest of this talk, we consider only the single band Hubbard model and enumerate some results.

5 Hubbard Model

Over a period of last thirty and odd years, this model has been chosen to be a minimal model for description of and transition to various ordered phases of correlated electronic systems. The model has a long history but there are very few exact results. However, there is a plethora of interesting, perturbative, variational, mean field, RPA and finite size numerical results. It is also true that in the same range of parameter space these results in general do not agree. After the discovery of high temperature superconductivity in cuprates and Anderson's assertion that the low energy physics of these superconductors is, again, given by the Hubbard model, there is a spurt of activity in this field. We therefore divide the summary of results in two parts [5, 8, 9, 12].

5.1 Hubbard Model, Pre-1986 results:

Before the high T_c frenzy the model has been applied mainly to correlation induced metal-insulator transition in half filled band and to the problem of magnetism in metals.[5, 8, 13, 14]. Almost all the standard techniques of quantum many body physics were used, viz. t-matrix approximation, equation of motion decoupling, coherent potential approximation, RPA, and the variational approach. Only in one dimension the model has been solved exactly. The results from these calculations cover some aspects of the correlation problem.

5.1.1 Metal-Insulator Transition:

The basic parameters of the model are the band filling ($n = 1$ means a half filled band), and the ratio U/zt, where z is number of nearest neighbours (zt is essentially the band width). For U vanishing we have a free electron gas. For a large U and if occupancy of lattice is confined to only one electron per site doubly occupied sites are highly suppressed and we have insulators Hubbard model has metal-insulator transition in it, by construction [13].

- For partially filled bands (and $n \neq 1$) the ground state is metallic for any strength of interaction and in any space dimension.

- In one dimension at half filling, the ground state is always insulating irrespective of the strength of the interaction. There is also a separation of spin and charge degrees of freedom. This is an exact result.

- $n = 1$, and in three dimensions there is a metal-insulator transition at $U \simeq zt$ Detailed nature of the transition, description of the insulating state etc. are not clear.

5.1.2 Magnetism:

The problem of magnetism in metals has been tackled from many directions within the model.

- In the insulating side of metal-insulator transition in three dimensions (for half filled band and for $U \gg zt$) the electrons are pinned and behave like local moments. These moments are antiferromagnetically coupled with $J \approx t^2/U$ [8].

- In the case of nesting of fermi surface or for a bipartite lattice there is always a spin density wave (SDW) ground state.

- Spin density wave also occurs when the spin susceptibility of band electrons has a peak at some wave vector, this SDW is metallic.

- In the metallic side when the density of states at the fermi energy ($\rho(\epsilon_F)$) is large, a mean field theory gives metallic ferromagnetism for $U\rho(\epsilon_F) > 1$ [5].

- In the extreme pathological but interesting case of one electron less than half filling, $U \rightarrow \infty$, there is a ferromagnetic ground state. This is known as the Nagaoka Ferromagnet [15]

5.1.3 Liquid ^{3}He:

Helium-3 is a Fermi liquid (helium nucleus has a spin 1/2), with a degeneracy temperature $\sim$ 5 K. In reality it behaves like a dense classical liquid for T $\geq$ .5 K and like a degenerate Fermi liquid below 0.2 K. At a pressure of about 34 Bar and at few mK it solidifies. And finally at very low temperatures T $\sim$ 0.001 - 0.0027 K it becomes superfluid. One can test various theories of correlation on it, because it is devoid of other "real life" problems like disorder, orbital degeneracy, lattice effects etc. There have been theoretical attempts to explain the low temperature behavior from two points of view phenomenologically. For detailed calculations the starting point is the Hubbard model in both theories [16].

- **Enhanced paramagnetism:** The (nuclear) spin susceptibility of ^{3}He varies between 10 - 25 times the free Fermi gas susceptibility, χ_P, depending on pressure. Because of the largeness of χ the liquid can be regarded as if it is near a ferromagnetic instability. Within the spin fluctuation theory, a theory which considers ^{3}He as a fermi liquid near a magnetic instability, the temperature dependence of many physical properties like spin susceptibility, specific heat is understood even at a quantitative level.

- **Incipient localization:** However, the velocity of sound is large in liquid ^{3}He. The compressibility at low temperatures is almost same as the compressibility of the solid phase. The liquid becomes sluggish at low temperatures before finally becoming a superfluid. One can consider ^3He as a liquid in the vicinity of a liquid to solid or the Mott-Hubbard "metal-insulator" transition. A theory based on this idea has been successful for understanding the pressure dependence of many properties.

- However, it turns out that these two approximation schemes give qualitatively different results when field dependence of susceptibility of polarised ^3He is calculated For example, spin fluctuation theory gives,

$$\chi(H) = \chi(0)(1 - \frac{1}{6}\frac{H^2}{\alpha(\alpha T_F)^2}), \tag{5}$$

that is, χ decreases with field, while the incipient localization model gives,

$$\chi(H) = \chi(0)(1 + \alpha\frac{9}{4}\frac{m^\star}{m}(\frac{m^\star/m}{1+F_0^a})^3\frac{H^2}{(T_F)^2}), \tag{6}$$

that is, χ increases. Here α is the susceptibility enhancement factor, $m^\star$ is effective mass and F_0^a is a Landau Fermi-Liquid theory parameter. Recent experiments on polarised liquid ^3He favour the spin fluctuation theory. However some recent results for Hubbard model in infinite dimensions for fermi liquid in the vicinity of metal to insulator seem to restore the spin fluctuation theory results [21].

5.2 Hubbard Model, Recent results:

It was recognised very early that the high T_c cuprates are doped Mott-Hubbard insulators and their physics lie essentially in CuO_2 planes. The work in high temperature superconductivity related to Hubbard model concentrated mainly on this aspect. strong correlation, vicinity of half filling and low dimensionality. However it was also difficult to ignore the weak coupling aspect of the problem. At present sustained effort is continuing in both directions.

5.2.1 Strong Coupling:

- For exact half filled band and for $U \rightarrow \infty$ we saw that the ground state is antiferromagnetic in three dimensions We have a spin -1/2 Heisenberg antiferromagnet. In two dimensions the quantum fluctuations around the classical Nèel state are important and have been been considered using various techniques. The consensus is that the ground state energy per site is $-0.66\ J$, and the staggered magnetisation is 0.3. At finite temperature the magnetic order disappears and the correlation length at low temperature follows the singular form $\xi(T) = C\exp(J/kT)$ [12].

- When holes are introduced, that is, when the band is slightly less than half filled, the relevant question is whether these holes move, how they interact amongst themselves and whether they form coherent pairs. In the strict anisotropic Ising case, holes do not move but are attached by a string force to their original positions. However, when spin fluctuations due to the transverse term are considered these strings are broken and holes can move depending on the relative strength of the Ising versus the transverse term [9].

- For a low density of these holes and for large correlations, $U \rightarrow \infty$, the Hubbard model can be canonically transformed to the $t - J$ model. This transformation was done earlier by Kohn and by Harris and Lange but has drawn considerable attention only recently [17].

$$\begin{aligned} H &= -t \sum_{\langle i,j \rangle} (1 - n_{i,-\sigma}) c^{\dagger}_{i,\sigma} c_{j,\sigma} (1 - n_{j,-\sigma}) + h.c. \\ &\quad + 4(t^2/U) \sum_{\langle i,j \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - n_i n_j/4) \end{aligned} \tag{7}$$

It is not possible to solve this model exactly either mainly because of the projection operators in the first term. Therefore, some drastic assumptions have been made on the first term and various mean field theories to RVB-, Chiral-, Flux- etc. phases have been proposed. The relative stability of these phases and their relevance to cuprates are still not clear.

- Large correlation imposes strong local restriction on the electronic occupancy: the electron occupancy is restricted to be zero or one independently at each site. Such a local restriction is hard to implement. They involve gauge symmetries. These have been formulated in terms of "Slave Fermion " and "Slave Boson " languages and a mean field theory is done. Within the slave Fermion language a mean field theory gives a rich phase diagram with ferromagnetic, antiferromagnetic, spiral and spin liquid phases [18]. A slave boson mean field theory is found to be equivalent to the Gutzwiller variational approach to the Hubbard model giving a metal to insulator transition [19].

- Is physics in two dimensions similar to that in One Dimension? In one dimension the Hubbard model and other equivalent fermionic models have been solved exactly long ago. It turns out that an electron added to the system can be thought of as a composite of a charge "e" and a spin- 1/2 excitation, two moving with different velocities. The ground state wave function for $U \to \infty$ can be written as a product of Slater determinant of noninteracting fermions and an exact wave function for one dimension Heisenberg chain. It has been argued by Anderson that this separation between charge and spin degrees of freedom is carried to higher dimensional correlated fermions also. For a collection of free fermions charge and spin degrees are not separable. However, for a Mott-Hubbard insulator, there is no charge motion but spin fluctuations can propagate. Similarly in one dimension (for $n \neq 1$) in the metallic side the single particle distribution function ($n(k)$) does not show a jump at the Fermi momentum but the slope of $n(k)$ has a power law singularity with exponent 1/8 for large U. This is known as a marginal fermi liquid behavior. It is not clear whether for a low density of holes in a Mott insulator in two dimensions a similar situation arises [20]

5.2.2 Weak Coupling:

- In two dimensions, with nearest neighbour hopping on a bipartite lattice (say, square lattice), for an exactly half filled band case the normal metallic state is unstable against the formation of spin density wave for any U. If a hole is introduced it perturbs the amplitude of SDW around it. If we add another hole, it may be energetically favourable for the two to be together and deform SDW locally. This is called spin bag. Is such a system stable? What happens to it when a large number of carriers are added? How is this state different from the string we talked about in the strong coupling case? [9]

- At a mean field level, one can think of the coupling between the two holes via antiferromagnetic spin fluctuations. This situation can arise in the strong as well as in the weak coupling case. In fact this problem was considered earlier for heavy fermion superconductors. This could lead to a d-wave pairing and to a weak coupling superconductivity.

There has been progress in other directions also, in particular there have attempts to solve the problem in infinite dimensions. The model can be mapped onto a single impurity model supplemented by a self consistency condition and the nature of metal insulator transition has been investigated [21].

6 Conclusion

There has been a major advancement in our understanding of correlated electronic systems during the last decade, inspite of the fact that even the minimal models have not been understood completely.

I am grateful to S.M. Bhattacharjee and H.N. Ghosh for making some useful comments on the manuscript.

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Indian J. Phys. **69A** (1), 65 – 75 (1995)

IJP A
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Magnetism and correlated electron systems

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Abstract: This review is concerned with the experimental results of some magnetic materials which exhibit unusual behaviour of the magnetisation with temperature compared to those for normal ferromagnetic, antiferromagnetic and ferrimagnetic compounds. The results of magnetic susceptibility, NMR and Mössbauer studies are discussed with a brief introduction of the application of NMR and Mössbauer spectroscopy for understanding the magnetic properties of solids.

Keywords: Magnetism, Low-dimensional system, Spin glass, Heavy fermions.

PACS nos: 75.50.-y

1. Introduction.

In recent years various types of magnetic materials have been discovered, showing unusual behaviour with temperature compared to those of normal ferromagnetic, antiferromagnetic and ferrimagnetic systems. Further, many new phenomena are observed in solids for which correlation effects among the electrons appear to be important. Some of these discoveries were made on systems where the low-dimensional aspects are essential, whereas, for other classes such as heavy fermions, strongly correlated electrons in three dimensional solids are concerned. The present review is concerned with the experimental results mainly of susceptibility, NMR and, Mössbauer studies of three types of magnetic materials viz., 1. low dimensional systems, 2. spin glass systems, and 3. heavy fermion systems. In section 2, a brief account will be given of how NMR and Mössbauer spectroscopy can provide information about the magnetic properties of solids. Sections 3, 4, and 5 will be devoted to the experimental results on above three types of systems.

2. NMR spectroscopy.

If we consider a solid containing atoms with non zero nuclear spin I, then it will have the magnetic dipole moment $\gamma\hbar I$, which will interact with the applied external magnetic field, H_o and the interaction Hamiltonian is $H = -\gamma\hbar I . H_0$ with energy eigen value $E=-\gamma\hbar H_0 m$. By application of a r.f. field of frequency, ν_o one can observe the transition between the Zeeman split levels. If in addition to the nuclear moments, there are atoms containing electronic moments, the nuclear moments can interact with these electronic moments through the hyperfine interaction $=-\gamma\hbar I H(t)$. The magnetic field, H(t) produced by the electrons at the nuclear site, is time dependent because of the fast flipping of the electronic spin due to various relaxation effects and exchange interactions. So, the total field at the nuclear site is $H=H_0+H(t)$. The time averaged part of H(t) produces a shift of the resonance line either towards low field or towards high field with respect to H_0 depending on the sign of $<H(t)>$. Further, $<H(t)>$ is proportional to the spontaneous magnetisation in the ordered state and the static susceptibility in the paramagnetic state. Fluctuating part of H(t) induces the spin- spin (T_2) and spin-lattice (T_1) relaxation times of the nucleus. The relaxation rates in this case are related to the Fourier transform of the electron spin pair correlation function $G(\mathbf{r}_{ij},t)$ by the relation[1]

$$T_i^{-1} = \sum_{\alpha}\sum_{q} C_{\alpha}^{i} A_{q}^{\alpha} S(q,\omega), (i = 1,2) \tag{1}$$

C_{α}^{i} depends on the nucleus and $S(q,\omega)$ is the Fourier transform of the electronic spin pair correlation function, $G(r_{ij},t)$. The q components of $S(q,\omega)$ are weighted by the A_q^{α} factor because the relaxation rates involve both the auto and pair correlation function of the electron spins. Therefore the study of the relaxation rates of the nucleus can provide information about the electron spin dynamics during the transition. Close to the magnetic ordering temperature (T_c) where the fluctuaion of the critical wave vector (q_c) dominates, the temperature dependent line width δH ($\sim T_2^{-1}$), in NMR is related to $\delta H \propto \epsilon^{-\gamma+\nu(d-z)}$ where d denotes the lattice dimensionality, γ and ν are the static critical exponents and z is the dynamic exponent, ϵ is the reduced temperature, $(T-T_c)/T_c$. So from the temperature dependent line width or the spin lattice relaxation rate near T_c, one can determine z, knowing the static exponents γ and ν, from other experiments.

Mössbauer Spectroscopy

The phenomena of the emission of gamma rays from nuclei and their resonance absorption by identical nuclei without any loss of energy due to recoil is known as Mössbauer effect. The recoil energy produced in gamma ray emmision is in fact taken up by the entire lattice. In a microscopic description, a certain fraction of the γ ray photon emitted by the nuclie will emerge without exciting any phonons. The time averaged

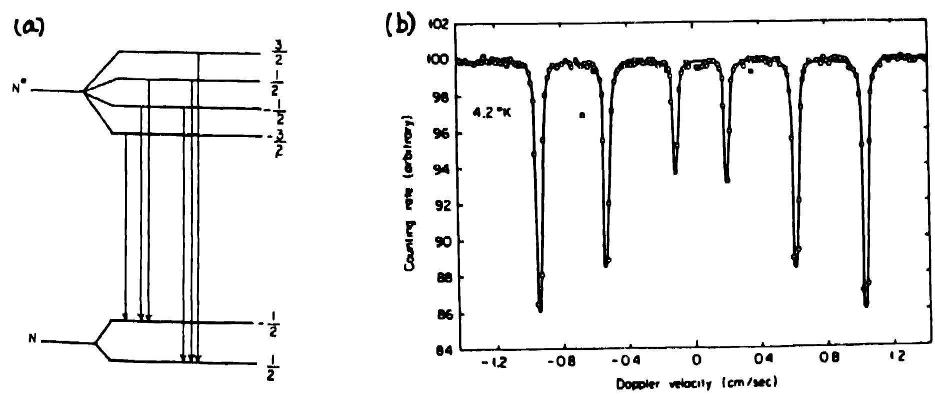

Fig.1 (a) Hyperfine structure in the nuclear excited state N* and ground state N of ^{57}Fe showing the six hyperfine transitions (neglecting the quadrupolar splitting) (b) Mössbauer spectrum of FeF_3 at 4.2K [1].